FILE 'HOME' ENTERED AT 16:36:44 ON 05 MAY 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 16:37:22 ON 05 MAY 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 MA

4 MAY 2005 HIGHEST RN 849790-35-8

DICTIONARY FILE UPDATES: 4

4 MAY 2005 HIGHEST RN 849790-35-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

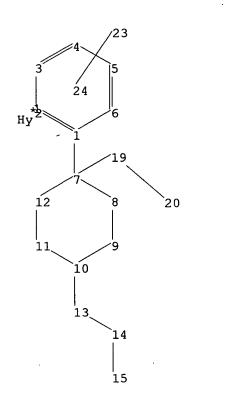
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09755021.str



*1 25

```
chain nodes :
13 14 15 19 20 23 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-7 7-19 10-13 13-14 14-15 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
10-13 14-15 19-20
exact bonds :
1-7 7-8 7-12 7-19 8-9 9-10 10-11 11-12 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 7 :
```

G1:0,S,N

G2:Ph,[*1]

STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1

STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sample

SAMPLE SEARCH INITIATED 16:37:44 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -3012 TO ITERATE

33.2% PROCESSED

1000 ITERATIONS

1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

56949 TO 63531

PROJECTED ANSWERS:

1 TO 164

1 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 16:37:52 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 61895 TO ITERATE

100.0% PROCESSED 61895 ITERATIONS 40 ANSWERS

161.54

SEARCH TIME: 00.00.02

L3

40 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE TOTAL

161.33

ENTRY SESSION

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 16:38:02 ON 05 MAY 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 5 May 2005 VOL 142 ISS 19 FILE LAST UPDATED: 4 May 2005 (20050504/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification. $\label{eq:case2} % \begin{substance} \begin{sub$

=> d 13
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L3 ANSWER 1 OF 40 REGISTRY COPYRIGHT 2005 ACS on STN 771463-77-5 REGISTRY ED Entered STN: 28 Oct 2004 CN 4-Morpholinecarboxamide, N-[3-[4-(5-fluoro-2-methoxyphenyl)-4-phenyl-1-piperidimyl]propyl]-3-oxo-5-phenyl-, (-)- (9CI) (CA INDEX NAME) FS STEREOSEARCH MF C32 H36 F N3 04 C1 COM 5R CA

Rotation (-).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

09/ 755,021

=> d 11 L1 HAS NO ANSWERS L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
Structure attributes must be viewed using STN Express query preparation.

=> s 13 L4 12 L3

=> d 14 1- ibib abs hitstr YOU HAVE REQUESTED DATA FROM 12 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 12
ACCESSION NUMBER:
DOCUMENT NUMBER:
100:1645698 CAPLUS
DOCUMENT NUMBER:
110:137:09
Self-organizing molecular field analysis on
als-adrenoceptor dihydropyridine antagonists
Li, Minyong: Du, Lupel; Wu, Binr Xia, Lin
Department of Medicinal Chemistry, China
Pharmaceutical University, Nanjing, 210009, Peop. Rep.

Bioorganic & Medicinal Chemistry (2003), 11(18), 3945-3951

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

3945-3951
COEDN: BMECEP; ISSN: 0968-0896
LISHER: Elsevier Science Ltd.
MENT TYPE: Journal
HUAGE: English
Salf-organizing mol. field anal. (SOMFA), a new three-dimensional quant.
structure-activity relationship (3-0-05AR) method is used to study the
correlation between the mol. properties and theela-AR biol.
activities of dihydropyridine derivs. The statistical result,
cross-validated q2 (0.690) and non cross-validated r2 (0.704) values, show
a good predictive shifty.
166808-19-1

166808-19-1

RE: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (self-organizing mol. field anal. on gla-adrenoceptor dihydropyridine antagonists)
166808-19-1 CAPLUS

IODBUS-19-1 CAPLUS
3,5-Pyridinedicarboxamide, 2-[(2-aminoethoxy)methyl]-1,4-dihydro-N3-[3-[4-(4-methoxy)menyl)-4-phenyl-1-piperidinyl]propyl]-6-methyl-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Title compds. [e.g., I; R = (un)substituted (hetero)aryl; Rl = H, (fluoro)alkyl, cyano, CO2RJ, etc.; R2 = H, akkyl, GN3, etc.; R3 = H, (fluoro)alkyl, etc.; R4 = e.g., (4-arylpiperidinopropyl)carbamoyl; X = O, S, (alkyl)mino] and analogs thereof were prepared Over 60 synthetic examples were provided. Thus 1,6-dihydro-5-(cyanoethoxycarbonyl)-4-ethyl-6-(4-nitrophenyl)-2-methoxypyrimiddine (prepared in 3 steps) was treated with 4-nitrophenylchloroformate (acylation at N1) followed by the corresponding substituted piperidine to give the N1 carboxamide intermediate. The 5-carboxamido derivative II. Thus, title compound II had pKi of 9.74 for binding at human ele receptors in vitro. Treatment of benign prostatic hyperplasia is a claimed use of the invention.

179480-91-22 179440-93-69
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses) (preparation of 1-(4-arylpiperidinopropyl)carbamoyl-2-piperidone-5-carboxylates and analogs as all antagonists)

179480-91-2 CAPLUS
5-Pyrinidinecarboxylic acid, 1,2,3,4-tetrabydro-1-{[[3-[4-(4-methyl-1-thioxo-, methyl ester (9CI) (CA INDEX NAME)

179480-95-6 CAPLUS 5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-[[[3-{4-(4-

L4 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 2001:560064 CAPLUS DOCUMENT NUMBER: 135:137519
TITLE: Preparation of \$ 1.00

INVENTOR (5):

135:137519
Preparation of 1-(4-arylpiperidinopropyl)carbamoyl-2-piperidone-5-carboxylates and analogs as alc antagonists
Nagarathnam, Dhanapalan; Chiu, George; Dhar, T. G. Murali; Wong, Wai C.; Marzabadi, Mohammad R.; Gluchowski, Charles; Lagu, Bharatr Niao, Shou Wu Synaptic Pharmaceutical Corp., USA
U.S., 67 pp., Cont.-in-part of U. S. Ser. No. 340,611, abandoned.
CODEN: USXXXM
Patent PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
						-						+			-		
US	6268	369			81		2001	0731		US 1	997-	8366	28		1	9970	516
WO	961	1846			A1		1996	0523		¥0 1	995-	US15	025		1	9951	116
	W:	AM,	AT.	AU.	BB.	BG.	BR.	BY.	CA.	CH,	CN.	CZ.	DE,	DK,	EE,	ES,	FI,
							KE.										
							NZ,										
		TH.															
	RW	KE,	LS.	MV.	SD.	SZ.	UG.	AT.	BE.	CH.	DE.	DK.	ES.	FR.	GB,	GR,	IE.
							SB.										
				TD.													
115	6241	2747					2001	0619		115 1	999-	2915	53		1	9990	414

US 1999-291553 US 2000-730458 US 1994-340611 WO 1995-US15025 US 1997-836628 US 1997-978682 19990414 20001205 B2 19941116 W 19951116 A1 19970516 A3 19971126 US 6727257 B1 20040427 PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 135:137519

ANSWER 2 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) methoxyphenyl)-4-phenyl-1-piperidinyl)propyl}amino]carbonyl]-4-methyl-6-(4-nitrophenyl)-2-oxo-, methyl ester (9CI) (CA INDEX NAME)

166809-56-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-(4-ary)piperidinopropyl)carbamoyl-2-piperidone-5carboxylates and analogs as elc antagonists)
166809-56-9 CAPLUS
1-Piperidinepropanamine, 4-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:874202 CAPLUS
134:29410
Freparation of oxazolidinones and related compounds as adrenergic all receptor antagonists
Lagu, Bherat Dhar, Tg Murali: Nagarathnam, Dhanapalan Jeon, Yoon T: Marzabadi, Mohammad R: Wong, Wai C: Gluchowski, Charles
PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corporation, USA
U.S. 74 DD.

PATENT ASSIGNEE(S): SOURCE: U.S., 74 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent English 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6159990 US 6620815 PRIORITY APPLN. INFO.:	A B1	20001212 20030916	US 1998-99225 US 2000-636518 US 1997-50096P US 1998-99225 A1	19980617 20000810 19970618 19980617

OTHER SOURCE(S): MARPAT 134:29410

Title compds. [I: X = 0, S: XI = 0, S. NH: R2 = H, (CH2)rXR3, CO2R3, alkyl, aminoalkyl, alkenyl, alkynyl, etc.; r = 1-4; R3 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl; R4 = (substituted) aryl, heteroaryl, aralkyl, heteroarylakyl, etc.; R5 = H, (substituted) aryl, aralkyl, heteroarylakyl, heteroaryl; adjacent R2R5 = aryl, heteroaryl, indianyl, tetrshydronaphthyl, cycloalkyl, heterocyclyl; Z = (substituted) acyl, alkenyl linker; R1 = (substituted) arylpiperidinyl, arylpiperarinyl, etc.], were prepared Thus, 4-(3,4-difluorophenyl)oxazolidin-2-one was stirred with NaH in THF/BHPA followed by addition of 1,5-dibromopentane to give 500 4-(3,4-difluorophenyl)-1-(5-bromopentyl)oxazolidin-2-one. this was refluxed with K2CO3 and 1-(2-methoxyphenyl)piperazine in dioxane to give 888 4-(3,4-difluorophenyl)-3-[5-[4-(2-methoxyphenyl)piperazin-1-yl]pertyl)oxazolidin-2-one. The latter bound to human alA, alb alb receptors with Ki = 0.5, 11, and 21, resp. 21848-46-89 21848-47-99 218451-03-99
218451-09-3P
R1: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); USES (Uses) (preparation of oxazolidinones and related compds. as adrenergic =1A receptor antagonists) AB

ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

218451-09-3 CAPLUS
1-Imidazolidi necarboxamide, 5-{3,4-difluorophenyl}-N-{3-[4-{2-methoxy-5-methylphenyl}-4-phenyl-1-piperidinyl]propyl]-2-oxo-, monohydrochloride
(SCI) (CA INDEX NAME)

216311-08-9

21631-08-9

RE: RCT (Reactant): RACT (Reactant or reagent)
(preparation of oxazolidinones and related compds. as adrenergic all receptor antagonists)
21631-08-9 CAPLUS
1-Piperidinepropanamine, 4-(2-methoxy-5-methylphenyl)-4-phenyl- (9CI) (CA INDEX RAME)

ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) 218449-46-8 CAPLUS 3-Oxazolidinecarboxamide, N-(3-[4-(5-bromo-2-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-4-(3,4-difluorophenyl)-2-oxo-, (+)- (9CI) (CA INDEX NAME)

218449-47-9 CAPLUS
3-Owazolidinecarboxamide, N-[3-[4-(5-bromo-2-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-4-(3,4-difluorophenyl)-2-oxo-, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+).

HC1

218451-05-9 CAPLUS 1-Imidazolidinecarboxamide, 5-(3,4-difluorophenyl)-N-(3-(4-(2-methoxy-5-methylphenyl)-4-phenyl-1-piperidinyl)propyl)-2-oxo- (9CI) (CA INDEX NAME)

ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

о || | (СН2) 3 — NH— С— ОВи- t

218449-45-7 CAPLUS 1-Piperidinepropanamine, 4-(5-bromo-2-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

218451-03-7 CAPLUS
1-Imidazolidinecarboxamide, 5-{3,4-difluorophenyl}-N-[3-{4-{2-methoxy-5-methylphenyl}-4-phenyl-1-piperidinyl]propyl]-2-oxo-3-(triphenylmethyl)-(SCI) (CA INDEX NAME)

ANSWER 3 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

REFERENCE COUNT:

THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT 46

ANSVER 4 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) cycloalkyl, cycloalkenyl; Y = 0, 5; R1 = specified (substituted) piperidinylalkylaminocarbonyl, piperaxinylalkylaminocarbonyl, etc., R2 = (substituted) aryl, heteroaryl; R3 = H, alkyl, fluoroalkyl, polyfluoroalkyl; N+etroaryl; R3 = H, alkyl, fluoroalkyl, polyfluoroalkyl; R4-R7 = H, (CH2)tYR8, (CH2)tCOZR8, (CH2)tCM, alkyl, Y = 0, S], were prepd. Thus, (+)-3-(3,4-difluorophenyl)-5-oxomorpholine-4-carboxylic acid 4-ntrophenyl ester (prepn. given) and 3-[4-(5-fluoro-2-methoxyphenyl)-4-phenylpiperidin-1-yl]propylamine were stirred at room temp. overnight in THF to give (+)-3-(3,4-difluorophenyl)-5-oxomorpholine-4-carboxylic acid 3-[4-(5-fluoro-2-methoxyphenyl)-4-phenylpiperidin-1-yl]propylamine stirred at room temp. overnight in THF to give (+)-3-(3,4-difluorophenyl)-5-oxomorpholine-4-carboxylic acid 3-[4-(5-fluoro-2-methoxyphenyl)-4-phenylpiperidin-1-yl)propylamine stirred at room temp. overnight in THF to give (+)-3-(3,4-difluorophenyl)-4-phenylpiperidin-1-yl)propylamine stirred at room temp. SEU (Riological study, unclassified); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Riological study); PREP (Preparation); USES (Uses) (preparation of morpholine derivs. as selective antagonists of ala receptors)
277295-67-7 CAPUS
4-Morpholinecarboxamide, 3-(3,4-difluorophenyl)-N-[3-[4-(5-fluoro-2-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-5-oxo-, monohydrochloride, (+)- (SCI) (CA INDEX NAME)

● HCl

277295-79-1 CAPLUS
4-Morpholinecarbomamide, N-{3-{4-(5-fluoro-2-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-3-oxo-5-phenyl-, monohydrochloride, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
DOCUMENT NUMBER:
131:58807
ITILE:
INVENTOR(5):
Lagu, Bharatr Nagarathnam, Ohanapalan; Tian, Dake;
Gluchowski, Charles
PATENT ASSIGNEE(5):
SOURCE:
PATENT ASSIGNEE(5):

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	01.																
PAT	ENT	NO.			KIN	D	DATE			APP	LICAT	ION	NO.		-	DATE	
#O	2000	0358	91		Al		2000	0622	,	RO	1999-	US 30	259			19991	217
	w:	AE,	AL,	AM,	AΤ,	ΑU,	ΑZ,	BA,	₿B,	BG	, BR,	BY,	CA,	CH,	CN	CR,	CU,
		CZ,	DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE	, GH,	GM,	HR,	ΗU,	ID	, IL,	IN,
		IS,	JΡ,	ΚE,	KG,	KP,	ĸR,	ΚZ,	ĿC,	LK	, LR,	LS,	LT,	LU,	ĽΛ	, ма,	MD,
		MG,	MK,	MN,	MW,	ΜX,	NO,	NZ,	PL,	PT	, RO,	RU,	5D,	SE,	SG	, SI,	SK,
		SL,	TJ,	TM,	TR,	TT,	ΤZ,	Uλ,	UG,	υz	, VN,	YU,	ZA,	Ζ¥,	AM	, AZ,	BY,
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		CG,	CI,	CH,	GA,	GN,	GW,	ML,	MR,	NE	, SN,	TD,	TG				
US	6218	390			Bl		2001	0417		บร	1998-	2135	39			19981	217
CA	2355	201		•	AA.		2000	0622		CA	1999-	2355	201			19991	217
EP											1999-						
	R:	AT,	BE,	CH,	DE,	DX,	ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE	, MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO										
JP	2002	5324	80		T2		2002	1002		JΡ	2000-	5881	52			19991	217
AU	7705	20			B2		2004	0226		ΑU	2000-	2197	3			19991	217
US	7705 6362	182			В1		2002	0326			2000-						
US	2002 6531	0687	37		A1		2002	0606		US	2001-	1726	3			20011	214
US	6531	471			B2		2003	0311									
US	2003	2120	62		A1		2003	1113		US	2003-	3860	83			20030	311
PRIORIT	Y APP	LN.	INFO	.:						US	1998-	2135	39		λ	19981	217
											1999-						
											2000-						
										US	2001-	1726	3		A1	20011	.214

OTHER SOURCE(S):

MARPAT 133:58807

Title compds. [I: II: III: W = O, S, NR8: R8 = H, alkyl, alkenyl, alkynyl,

ANSWER 4 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

● HCl

277295-81-5 CAPLUS
4-Morpholinecarboxamide, 3-{3,4-difluorophenyl}-N-[3-[4-{5-fluoro-2-methoxyphenyl}-4-phenyl-1-piperidinyl]propyl]-2-methyl-5-oxo-, monohydrochloride, (2R, 3R)-rel-(+)- (9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

● HC1

277296-20-5 CAPLUS
4-Morpholinecarboxamide, 3-{3,4-difluorophenyl}-N-{3-{4-(5-fluoro-2-methoxyphenyl}-4-phenyl-1-piperidinyl]propyl}-5-oxo-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

277295-95-1F 277296-11-4F

277295-95-19 277296-11-4P

RI: RCT (Reactant) : SPM (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of morpholine derive. as selective antagonists of ala receptors)

277295-95-1 CAPLUS

27/23-3-1 CARDOS 1-Piperidinepropanamine, 4-(5-fluoro-2-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

277296-11-4 CAPLUS
Carbantc acid, [3-(4-(5-fluoro-2-methoxyphenyl)-4-phenyl-1-piperidinyl)propyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

L4 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1999:662323 CAPLUS DOCUMENT NUMBER: 132:44482

ACCESSION NUMBER:
1999:662323 CAPLUS
DOCUMENT NUMBER:
102:44462
TITLE:
Design and synthesis of novel dihydropyridine alpha-1A
antagonists
ANTHOR(S):
Marrabadi, Mohammad R.; Hong, Xingfang, Nagarathnam,
Dhanapalan, Niao, ShouMu; Chiu, George; Wong, Wai C.;
Wetzel, John M.; Fang, James; Forray, Carlos; Chen,
Tsing B.; O'Malley, Stacey S.; Chang, Raymond S. L.;
Gluchowski, Charles
CORPORATE SOURCE:
Department of Chemistry, Synaptic Pharmaceutical
Corporation, Paramus, NJ, 07652, USA
SOURCE:
Bioorganic & Medicinal Chemistry Letters (1999),
9(19), 2843-2848
CODEN: BRILES; ISSN: 0960-894X
Elsevier Science Ltd.
DOCHENT TYPE:
DOCHENT TYPE:
JOURNAL
AB A series of analogs of SNAP 5150 containing heteroatoms at C2 or C6
positions
is described. Herein, the authors report that the presence of alkyl
substituted heteroatoms at the C2(6)-positions of the dihydropyridine are
well tolerated. In addition, SNAP 5399 inhibited the phemylephrine induced
contraction of dog prostate tissue with a Rb of 1.5 m and showed a Rb
(DBP, dogs, pg/kg)/Rb (TUP, dogs, pg/kg) ratio of 14.872.5.

Ti 16600-19-1
Ri: BAC (Biological activity or effector, except adverse): BSU (Biological
study, unclassified): TBU (Therapeutic use): BIOL (Biological study): USES
(design and synthesis of novel dihydropyridine alpha-1A antagonists in
relation to structure and inhibition of preserve.

(Uses)
(design and synthesis of novel dihydropyridine alpha-lA antagonists in relation to structure and inhibition of prostate contraction and hioavailability)
166808-19-1 CAPLUS
3,5-Pyridinedicarboxamide, 2-[(2-aminosthoxy)methyl]-1,4-dihydro-N3-[3-[4-de-methoxyhenyl]-4-phenyl-1-piperidinyl]propyl]-6-methyl-4-[4-nitrophenyl]- (SCI) (CA INDEX NAME)

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	KIND DATE					
WO 9857940	A1 19981223	WO 1998-U512668				
W: AL, AM, AT,	AU, AZ, BA, BB, BG,	BR, BY, CA, CH, CN,	CU, CZ, DE,			
DK. EE. ES.	FI. GB, GE, GH, GM,	GW, HU, ID, IL, IS,	JP, KE, KG,			
KP. KR. KZ.	LC. LK. LR. LS. LT.	LU. LV. MD. MG. MK.	MN. MW. MX.			
NO. NZ. PL.	PT, RO, RU, SD, SE,	SG. SI. SK. SL. TJ.	TM. TR. TT.			
	VN. YU. ZW. AM. AZ.					
	LS. MW. SD. SZ. UG.					
	GR, IE, IT, LU, MC,					
	ML. MR. NE. SN. TD.		01, 00, 01,			
	AA 19981223					
AU 9881498	A1 19990104	AU 1998-81498	19980617			
AU 740064	B2 20011025					
EP 988295	A1 20000329	EP 1998-931350	19980617			
	DE, DK, ES, FR, GB,					
IE. FI	,,,,					
	T2 20020219	JP 1999-50477R	19980617			
		US 1997-877846				
PRIORITY APPLN. INFO.:						
,		WO 1998-U512668	W 19980617			
OTHER SOURCE(S):	MARPAT 130:81508					

This invention is directed to oxazolidinone compds. which are selective antagonists for human all receptors. These compds. lower intraocular pressure, inhibit cholesterol synthesis, relax lower urinary tract tissue, and are useful in the treatment of benign prostatic hyperplasia, impotency, cardiac arrhythmia etc. Thus, 4-(3,4-difluorophenyl)oxazolidinone was treated with 1,5-dibromopentane,

ANSYER 6 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) followed by 1-(2-methoxyphenyl)piperazine to give the oxazolidinone I which had a binding affinity for human all receptors of 0.5 nM. 218449-64-69 218449-64-79 218451-03-7P RD: RCT (Reactant), SPN (Synthetic preparation), PREP (Preparation), RACT (Reactant)

(Reactant or reagent)
(preparation of heterocyclic substituted oxazolidinones for use as

selective

ctive
antagonists for human alk receptors)
218449-44-6 CAPUS
Carbamic acid, [3-[4-(5-bromo-2-methomyphenyl)-4-phenyl-1piperidinyl]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

218449-45-7 CAPILIS

1-Piperidinepropanamine, 4-(5-bromo-2-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

218451-03-7 CAPLUS
1-Imidazolidinecarboxamide, 5-{3,4-difluorophenyl}-N-{3-{4-(2-methoxy-5-methylphenyl}-4-phenyl-1-piperidinyl}propyl}-2-oxo-3-(triphenylmethyl)-(9CI) (CA INDEX NAME)

ANSWER 6 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT 218449-47-99 218451-09-39
RL: SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses)
(preparation of heterocyclic substituted oxazolidinones for use as selective
antagonists for human all receptors)
RN 218449-47-9 CAPLUS
CN 3-Oxazolidinecarboxamide, N-[3-[4-(5-bromo-2-methoxyphenyl)-4-phenyl-1-piperidinyl]proxyl]-4-(3,4-difluorophenyl)-2-oxo-, monohydrochloride, (+)-(9CI) (CA INDEX NAME)

Rotation (+).

● HCl

218451-09-3 CAPLUS
1-Imidazolidinecarboxamide, 5-{3,4-difluorophenyl}-N-{3-{4-(2-methoxy-5-methylphenyl)-4-phenyl-1-piperidinyl}propyl}-2-oxo-, monohydrochloride
(9CI) (CA INDEX NAME)

ANSWER 6 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT

218449-46-8P 218451-05-9P
RL: RCT (Reactant): SPN (Synthetic preparation): THU (Therapeutic usa):
BIOL (Biological study): PREP (Preparation): RACT (Reactant or reagent):
USES (Uses)

(preparation of heterocyclic substituted oxazolidinones for use as selective

ctive
analogorists for human wlA receptors)
218449-46-8 CAPLUS
3-Owazolidinecarbowamide, N-[3-[4-(5-bromo-2-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-4-(3,4-difluorophenyl)-2-oxo-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

218451-05-9 CAPLUS
1-Imidazolidimecarboxamide, 5-(3,4-difluorophenyl)-N-[3-[4-(2-methoxy-5-methylphenyl)-4-phenyl-1-piperidinyl)propyl)-2-oxo- (9CI) (CA INDEX NAME)

ANSWER 6 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1998:764290 CAPLUS DOCUMENT NUMBER: 130:25077
TITLE: Preparation 130:25077
Preparation of piperidinylpropylaminocarbonyldihydropy rimidones and related compounds as selective adrenergic alA receptor antagonists.
Wong, Vai C.; Lagu, Bharati Nagarathnam, Dhanapalan; Marzabadi, Mohammad R.; Gluchowski, Charles Synaptic Pharmaceutical Corporation, USA PCT Int. Appl., 314 pp. CODEM: PIRMID2

INVENTOR (5):

PATENT ASSIGNEE(S):

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

11111111	11110																
P	ATENT	NO.			KIND DATE				APPL	ICAT		DATE					
-						-							_				
v	o 9851	311			A2 19981119			1	WO 1	998-		19980515					
u	O 9851	311			A3		1999	0114									
	W:	AL,	AM,	AT,	AU,	λZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	Cυ,	CZ,	DE,
		DK,	EE,	ES,	FI,	GB,	GE,	GH,	GM,	GW,	ΗU,	ID,	IL,	IS,	JP,	KE,	KG,
		KP,	KR,	KZ,	LC,	LK,	LR.	LS,	LT.	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,
		NO.	NZ,	PL,	PT,	RO,	RU,	SD.	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,
		UA,	UG,	UZ,	VN,	YU,	Z¥.	AM.	AZ,	BY,	KG,	KZ,	MD,	RU,	ŤJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MV.	SD.	SZ.	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,	ES,
		FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	Œ,	CI,
		CH,	GΑ,	GN,	ML,	MR,	NE,	SN,	TD,	TG							
u	5 6245	773			B1		2001	0612		US 1	997-	8580	17		1	9970	516
A					A1		1998	1208		AU 1	998-	7687	2		1	9980	515
t	US 2002010186						2002	0124		US 2	001-	B 555	97		2	0010	515
PRIORI	PRIORITY APPLN. INFO.:									US 1	997-	8580	17		A 1	9970	516
										US 1	996-	1780	1P		P 1	9960	516
										wn 1	QQR-	11210	OR2		4 1	ORPP	515

MARPAT 130:25077 OTHER SOURCE(S):

Title compds. [I, II, III; A = specified (substituted) (hetero)aryl; X = 5, 0, NR3; RI = H, NO2, cyano, alkyl; fluoroalkyl, alkenyl, alkynyl, cycloalkyl, fluorocycloalkyl, cycloalkyl, fluoroalkyl, alkenyl, RR3)2; R2 = H, alkyl; hydroxyalkyl, alkoxyalkyl, aminoalkyl, fluoroalkyl, alkenyl, alkynyl, cycloalkyl, fluorocycloalkyl, cycloalkylalkyl, cyano, OR3, etc., R3 = H, alkyl, fluoroalkyl, alkenyl, alkynyl, cycloalkyl, fluorocycloalkyl, cycloalkenyl, R4 = specified substituted heterocyclylphperidinylalkyl, etc., n = 0-5, were prepared I are useful for lowering intraocular pressure, inhibiting cholesterol

ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

200051-57-6 CAPLUS
5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4(methoxymethyl)-1-[[[3-[4-(2-methoxy-5-methylphenyl)-4-phenyl-1piperidinyl)propyl]amino]carbonyl]-2-oxo-, methyl ester,
monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

● HCl

216310-39-3 CAPLUS
5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1[[[3-[4-(4-hydroxyphenyl)-4-phenyl-1-piperidinyl]propyl]amino]carbonyl]-4
methyl-2-axo-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) synthesis, relaxing lower urinary tract tissue, treatment of benign prostatic hyperplasia, impotency, cardiac archythmia, etc. Thus, (+)-5-carboxamido-4-cthyl-1-[N-[3-(4-methoxycarbony]-4-phenylpiperidin-1-yl)propyl])carboxamido-6-(4-nitrophenyl)-2-oxo-1,2,3,6-tetrahydropyrimidine (prepn. given) bound to human all receptors with pKi = 9.74.
200050-42-69 200050-45-99 200051-01-09
200051-37-69 216310-39-39 216311-38-59
RL: BAC (Biological activity or effector, except adverse): BSU (Biological study, unclassified): SPN (Synthetic preparation): TBU (Therapeutic use): BIOL (Biological activity): PREP (Preparation): USES (Uses)
(preparation of piperidinylpropylaminocarbonyldihydropyrimidones as selective adrenergic all receptor antagonists)
200550-42-6 CAPLUS
5-Pyriatidinecarboxylic acid, 1,2,3,6-tetrahydro-1-[[[3-[4-(4-methoxyphenyl]-4-phenyl-1-piperidinylpropyl]aminocarbonyl]-4-methyl-6-(4-nitrophenyl)-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

200050-45-9 CAPLUS

20090-43-9 cartol scid, 1,2,3,6-tetrahydro-1-[[[3-[4-(4-methoxphenyl)]-4-phenyl-1-piperidinyl]propyl]amino]carbonyl]-4-methyl-6-(4-ntroxphenyl)-2-oxo-, methyl-seter (9CI) (CA INDEX NAME)

200051-01-0 CAPLUS
5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4(methoxymethyl)-1-[[[3-[4-[2-methoxy-5-methylphenyl)-4-phenyl-1piperidinyl]propyl]amino|carbonyl]-2-oxo-, methyl ester, (+)- (9CI) (CA
INDEX NAME)

Rotation (+).

ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

216311-38-5 CAPLUS
5-Pyriaidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4(methoxymethyl)-1-[[[3-[4-(2-methoxy-5-methylphenyl)-4-phenyl-1piperidinyl]propyl]amino]carbonyl]-2-oxo-, methyl ester (9CI) [CA INDEX
NAME)

166809-56-9P 216311-08-9P 216311-32-9P

loadur-se-wy fieli-us-wy 210311-32-wy
RE: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation of piperidinylpropylaminocarbonyldihydropyrimidones as
selective adrenergic all receptor antagonists)
16809-56-9 (APLUS

166809-56-9 CARLOS 1-Piperidinepropanamine, 4-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX

216311-08-9 CAPLUS 1-Piperidinepropanamine, 4-(2-methoxy-5-methylphenyl)-4-phenyl- (9CI) (CA

ANSWER 7 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN INDEX NAME) (Continued)

216311-32-9 CAPLUS
Carbanic acid, [3-(4-(2-methoxy-5-methylphenyl)-4-phenyl-1-piperidinyl)propyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB The dihydropyridine derivs. [I; Rl = linear or branched alkyl, alkoxyalkyl, aralkyl; R2, R4 = H, linear or branched alkyl, akoxyalkyl, acyl; R5, R6 = H, CH, Cl, Br, F, NO2, CF3, cyano, NEZ, etc.; R7, R8 = H, cyano, CF3, OH, alkoxy, etc.; Y = Cl-5 alkylene, C4-8 alkylene intercupted by O, alkenylene, alkynylene, etc.; Z = 0, NH, CH2], useful in treating benign prostatic hyperplasia, inhibition of cholesterol synthesis, and reduction in intraocular pressure, are prepared and formulated. Amidation of carboxylic acid II (preparation given) with 3-(4,-4-diphenylpiperidino)propylamine in refluxing CH2Cl2 gave 58.84 title compound (1)-III, which showed Ki of 1.9 nmol/kg.in reducing urethral pressure in vivo in dogs.

IT 166807-19-8P 166800-139-8P 166800-40-8P 166807-49-PP 166800-1-19-B 166800-1-19-B; NSONO-4-2P 16-MENTAL NS

L4 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
1998:414735 CAPLUS
129:67709
Dihydropyridine derivatives for treatment of benign prostatic hyperplasia
INVENTOR(5):
Gluchowski, Charles: Wetzel, John M.; Chiu, George: Marzabadi, Nohammed R.; Wong, Wai C.; Nagarathnam, Dhanapalan
Synaptic Pharmaceutical Corporation, USA
U.S., 160 pp., Cont.-in-part of U.S. Ser. No. 166,367, abandoned.
CODEN: USXXXM
DOCUMENT TYPE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: Patent English 2

FAIRM INFORMATION.								
PATENT NO.		APPLICATION NO.						
US 5767131		US 1996-211764	19960223					
		WO 1994-US3852						
WO 9422829			13340403					
			me my cn cm					
		CH, CN, CZ, DE, DK,						
		LU, LV, MD, MG, MN,						
		SK, TJ, TT, UA, US,						
		GB, GR, IE, IT, LU,						
BF, BJ, CF,	CG, CI, CM, GA,	GN, ML, MR, NE, SN,	TD, TG					
2A 9402360	A 19950522	ZA 1994-2360 US 1998-98699	19940405					
US 6211198	B1 20010403	US 1998-98699	19980615					
US 6310076	B1 20011030	US 2000-588973	20000607					
US 2002193599		US 2001-972801						
	B2 20030819							
PRIORITY APPLN. INFO.:		US 1993-43212	B2 19930405					
PRIORITI APPLA. INTO		US 1993-120169						
		US 1993-166367						
		WO 1994-US3852						
		US 1993-166308						
		US 1996-211764						
		US 1998-98699						
		US 2000-588973	A3 20000607					

OTHER SOURCE(S): MARPAT 129:67709

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

HC1

166807-35-8 CAPLUS
3,5-Pyridinedicarboxamide, 1,4-dihydro-N-{3-[4-(4-methoxyphenyl)-4-phenyl-rpiperidinyl]ropyl]-2,6-dimethyl-4-(4-nitrophenyl)-, monohydrochloride
(9C1) (CA INDEX NAME)

166807-43-8 CAPLUS
3,5-Pyridinedicarboxamide, 2,6-diethyl-1,4-dihydro-N-[3-[4-(4-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-N'-methyl-4-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

166807-47-2 CAPLUS
3,5-Pyridinedicarboxamide, N,2,6-triethyl-1,4-dihydro-N'-[3-[4-(4-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-4-(4-nitrophenyl)- (9CI)
(CA INDEX NAME)

166808-17-9 CAPLUS
3,5-Pyridinedicarboxamide, 2-[(2-azidoethoxy)methyl]-1,4-dihydro-N3-[3-[4-(4-methoxy)henyl)-4-phenyl-1-piperidinyl)propyl]-6-methyl-4-(4-itrophenyl)- (9CI) (CA INDEX NAME)

166808-19-1 CAPLUS
3,5-Pyridinedicarboxamide, 2-[(2-aminoethoxy)methyl]-1,4-dihydro-N3-[3-[4-

L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:
DOCUMENT NUMBER:
11997:752040 CAPLUS
129:61520
Preparation of dihydropyrimidine derivatives as selective antagonists for human dlA-adrenergic receptors.

INVENTOR(5): Wong, Wai C., Lagu, Bharat, Nagarathnam, Dhanapalan, Marzabadi, Mohammad R., Gluchowski, Charles Synaptic Pharmaceutical Corporation, USA
PATENT ASSIGNEE(5): Synaptic Pharmaceutical Corporation, USA
PCT Int. Appl., 271 pp.
CODEM: PIXMOZ
DOCUMENT TYPE: Patent
LNGUAGE: PIXMOZ
PATENT INFORMATION: 2

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PRI

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		956					1997	1120			1997-						
											BY,						
											IS.						
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	R¥:										CH.	DE.	DK.	ES.	FI.	FR.	GB.
											BJ,						
							TG		,								
CA	225									CA	1997-	2253	962		1	9970	516
All	973	082			A1		1997	1205		All	1997-	3008	2		•	9970	516
All	727	72			R2		2001	0104					-				
										JP '	1997-	5411	46		1	9970	516
		1185									1997-						
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		IE.		٠		,			,		,		,	,	,	,	,
115	200	20101			A1		2002	0124		115	2001-	8555	97		-	20010	515
		LN.			~~		2001				1996-						
,KI 1			****	••							1996-						
											1997-					9970	
											1997-					9970	

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The title compds. [I, II, and III; A = (un) substituted Ph, pyridyl, IH-iaidazolyl, or 1-iaidazolyl, etc.; X = H, NO2, cyano, linear or branched C1-7 alkyl, mono- or polyfluoroalkyl, linear or branched C2-7 alkyl, mono- or polyfluoroalkyl, linear or branched C2-7 alkyl, grand, compositivelyl, linear or branched C2-7 alkyl, hydroxyalkyl, alkowyalkyl, asinoalkyl, sono- or polyfluorocycloalkyl, mono- or polyfluorocycloalkyl, mono- or polyfluorocycloalkyl, alkowyalkyl, alkowyalkyl, asinoalkyl, or cycloalkyl, crandom C2-7 alkenyl or alkymyl, C3-10 cycloalkyl-C1-10 alkyl, C3-10 cycloalkyl-C1-10 alkyl, C3-10 cycloalkyl-C1-10 mono- or polyfluorocycloalkyl, cyano, CHZNJ, CHZY (CHZ) pNHJJ, (CHZ) NHJJ, C3-10 cycloalkyl, C3-10 cycloalkyl, C3-10 cycloalkyl, C3-10 cycloalkyl, cyano, CHZNJ, CHZY (CHZ) pNHJJ, (CHZ) nHJJ, cyano, CHZNJ, CHZY (CHZ) pNHJJ, (CHZ) nHJJ, cyano, CHZNJ, CHZY, CHZ) pNHJJ, (CHZ) nHJJ, cyano, CHZNJ, CHZY, CHZ) pNHJJ, (CHZ) nHJJ, cyano, CAZNJ, CHZY, CHZ) pNHJJ, (CHZ) nHJJ, cyano, CHZNJ, CHZY, CHZ) pNHJJ, (CHZ) nHJJ, cyano, CHZNJ, cyano, c

ANSWER 8 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (4-methoxyphenyl)-4-phenyl-1-phenidinyl)propyl}-6-methyl-4-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

166809-56-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of dishydropyridine derivs. as drugs)
166809-56-9 CAPLUS
1-Piperidinepropanamine, 4-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
F, linear or branched C1-7 alkyl, mono- or polyfluoroalkyl, linear or
branched alkyl C2-7 alkenyl or alkynyl, N(R3)2, NO2, etc., R5, R7 = H, F,
Cl. Br, iodo, COR3, COR3, COR3, COR(R)2, cyano, NO2, N(R)2, OR3, SR3,
(CH2)pSR3, etc., R6 = H, linear or branched C1-7 alkyl,
hydroxyalkyl, minoalkyl, alkowyalkyl, mono- or polyfluoroalkyl, C3-7
cycloalkyl]. This invention is also celated to uses of these compds for
lowering intraocular pressure, inhibiting cholesterol synthesis, relaxing
lower urinary tract tissue, the treatment of benign prostatic hyperplasia,
impotence, cardiac archythmia and for the treatment of any disease where
the antagonism of the allx receptor may be useful. The invention
further provides a pharmaceutical compn. comprising a therapeutically
acceptable carrier. Thus, a mixt. of 1-(5-chloropentyl)-6-(3,4difluorophenyl)-1,6-dhydro-2,4-dimethyl-5-methoxycarbonylpyrimidine
(preps. given), 4-methoxycarbonyl-4-phenylpiperidine, K2CO3, and NaI, and
affinities at cloned human aid, alb, and ala receptors
with pKi values of 6.17, 6.32, and 8.99, rep.
200050-42-69 200050-45-99 200050-61-39
200051-0109 200051-37-69
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study), unclassified) SFN (Synthetic preparation); TBU (Therapeutic use);
BIO, (Biological study); PREP (Preparation); USES (Uses)
(preparation of dihydropyrimidine deriva, as selective antagonists for
all-adrenergic receptors for disease treatment)

alA-adrenergic receptors for disease treatment)
200050-42-6 CAPLUS

5-Dyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-1-[[{3-[4-(4-methoxyherol-1-[4-methoxyherol-1-[4-methoxyherol-1-4-methoxyherol-1-4-methoxyherol-1-2-thioxo-, methyl abstr [9cr) (CA INDEX NAME)

200050-45-9 CAPLUS

200030-43-9 Armylic acid, 1,2,3,6-tetrahydro-1-[[{3-[4-(4-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]anino|carboxyl-4-methyl-6-(4-ntrophenyl)-2-oxo-, methyl ester (9CI) (CA INDEX MADE)

ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) 200050-81-3 CAPLUS 5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-1-[[[3-[4-4-hydroxyphenyl]-4-phenyl-1-piperidinyl]propyl]amino]carbonyl]-2-oxo-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

• HCl

200051-01-0 CAPLUS
5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4(methoxymethyl)-1-[[[3-[4-(2-methoxy-5-methylphenyl)-4-phenyl-1piperidinyl]propyl]amino]carbonyl]-2-oxo-, methyl ester, (+)- {9CI} (CA
INDEX NAME)

200051-57-6 CAPLUS
5-Pyrimidinecarboxylic acid, 6-(3,4-difluorophenyl)-1,2,3,6-tetrahydro-4(methoxymethyl)-1-[[[3-[4-(2-methoxy-5-methylphenyl)-4-phenyl-1piperidinyl]propyl]amino]carbonyl]-2-oxo-, methyl ester,
monohydrochloride, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

L4 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

200052-35-3 CAPLUS
Carbamic acid, [3-[4-(5-methoxy-2-methylphenyl)-4-phenyl-1piperidinyllpropyl]-, 1.1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

166809-56-9P 200052-34-2P 200052-35-3P RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent) (preparation of dihydropyrimidine derivs. as selective antagonists for

all-adrenergic receptors for disease treatment)
166809-56-9 CAPLUS
1-Piperidinepropanamine, 4-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

200052-34-2 CAPLUS 1-Piperidinepropanamine, 4-(5-methoxy-2-methylphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
1996:473181 CAPLUS
125:142759
125:142759
Preparation of 1-(4-arylpiperidinopropyl)carbamoyl-2-piperidone-5-carboxylates and analogs as alc antagonists
Nagarathnam, Dhanapalan; Chiu, George; Dhar, T. G. Murali Yong, Wai C.; Marzabadi, Mohammad R.;
Gluchowski, Charles; Lagu, Bharat; Miao, Shou Wu
Symptic Pharmaceutical Corporation, USA
PCT Int. Appl., 229 pp.
CODEM: PIXKD2
PATENT ASSIGNEE(S):
English
FAMILY ACC. NUM. COUNT:
4

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	ENT I	ю.			KINI	•	DATE			APP	LIC	CATI	ON 1	NO.		Di	TE		
20	9614	146			A1		1996	0523		¥0	199	95-0	JS150	025		19	951	116	
	W:	AM.	AŤ.	AU.	BB.	BG.	BR.	BY.	CA.	CH	. (CN.	CZ,	DE,	DK,	EE,	ES,	FI,	
		GB.	GE.	HU.	IS.	JP.	KE,	KG,	KP,	KR	. 1	ΚZ,	LK,	LR,	LT,	LU,	LV,	MD,	
		MG,	MN,	MV.	MX,	NO,	NZ,	PL,	PT,	RO	, 1	RU,	SD,	SE.	SG,	SI,	SK,	TJ,	
		TM,																	
	RW:	KE,	LS,	MV,	SD,	SZ,	UG,	AΤ,	BE,	CH	. 1	DE,	DK,	ES,	FR,	GB,	GR,	IE,	
						PT,	SE,	BF,	BJ,	CF	. (Œ,	CI,	CH,	GA,	GN,	ML,	MR,	
			SN,	TD,	TG														
CA	2205	384			λλ		1996	0523		CA	19	95-7	2205	384		1	9951	116	
CA	2205 2205 9642 7146 7908	384			C		2004	0629											
λU	9642	398			λl		1996	0606		ΑU	19	96-	1239	a		1	995 I	116	
AU	7146	40			В2		2000	0106											
EP	7908	26			A1		1997	0827		EP	19	95-:	940/	48		1	9951	110	_
	R:	AT,	BE,	CH,	DE,	DK,	E5,	FR.	GB,	GR		IE,	IT,	. LL.	LU,	ML,	NL,	PT,	Э.
CN	1173	132			Α.		1998	0211		CN	19	95-	19/3	48		1	3321	110	
JP	1051	0247			TZ		1998	1006		JP	19	96-	2103	54		1	3321	110	
JΡ	R: 1173 1051 3200 9509 7794 2237 9717	070			82		2001	0820											
BR	9509	700			Α.		1998	1103		BR	19	95-	9 / 00			- 1	7931	116	
HU	7794	1			AZ		1998	1228		HO	13	28-	1222	~~.		- :	223 <i>t</i>	116	
CA	2237	7/4			^^		1997	0522		<u>بم</u>	13	30-	2231	. 73		- :	2201	115	
WO	9717	969			- A1		BA,	0522		80	13	30-	0210	3/3	~.	~.'	3201	113	
	٧:						GE,												
		UK,	EE,	E5,	F1,	GB.	LV,	HU,	10,	12		JP,	KE,	MV,	Mr.	NT,	DI.	DT,	
		LK,	LH,	LS,	LT,	ш,	SK,	MD,	MG,			MN,	ne,	ma,	no,	ne,	117	VA.	
		RU,	50,	5E,	20,	21,	MD,	10,	10,			11,	UM,	uu,	υ3,	03,	UL,	V 14,	
		AM,	AZ,	ы,	KG,	KZ,	UG,	KU,	10,		:	D.W.	DIF	TC	77.7	WD.	CB	CB	
	K#:	KE,	ъ,	mw,	ου,	34,	PT,	AI,	DE,	, C.	١,	CP.	or.	CI.	~	GA,	GN,	MI.	
		***	****			=-													
		MK,	NE,	ъN,	10,	16	1007	0606			10	07-	1055			٠,	9961	115	
<u>۸</u>	3110	07			D.7		1000	1223		AU	.,	,,-	1000			•	,,,,		
AU	7142	612					1007	0721		78	10	06-	0612			,	9961	115	
4A	9710 7142 9609 8667	012			٠,		1000	0121		ED.	19	96-	9414	06		i	9961	115	
EF	7007	37	92	~	U.	DA	PC	PB	GR		,	TT	1.1	11.1	NT.	SE.	MC.	PT,	
10	2000	5004	20		77		2000	0110		.TD	10	97-	5191	57		1	9961	115	
VF	0703	226	,,				1007	0701		NO.	10	07-	2236			î	9970	515	
NO.	0702	007			•		1007	0714		P7	10	07-	2087			i	9970	1515	
t r	6760	360			<u>،</u>		2001	0731		115	19	97-	8366	2A		i	9970	516	
116	2000 9702 9702 6268 5942 6228 6248	517			21		1900	0.31		us	19	97-	9786	82		- 1	9971	126	
us	3344	257			21		2001	0508		115	19	99-	5878	2		1	0001	110	
1116																			

L4 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN US 6727257 B1 20040427 US 2000-730458 PRIORITY APPLN. INFO.: US 1994-340611 W0 1995-US15025 US 1996-648770 W0 1996-US18573 US 1997-978682 US 1997-978682 (Continued) 20001205 A 19941116 W 19951116 A 19960516 W 19961115 OTHER SOURCE(S): MARPAT 125:142759

Title compds. [e.g., I: R = (un)substituted (hetero)aryl: Rl = H. (fluoro)alkyl, cyano, .CO2R3, etc.: R2 = H. alkyl. OR3, etc.: R3 = H. (fluoro)alkyl. etc.: R4 = e.g. (4-arylpiperidinopropyl)carbamoyl: X = O. S. (alkyl)aino] were prepared Thus, title compound II had pRi of 9.74 for binding at human elc receptors in vitro. 179480-91-29 179480-95-69
RL: RAC (Slological activity or effector, except adverse): BSU (Biological actudy, unclassified): SPN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREF (Preparation): USES (Uses) (preparation of 1-(4-arylpiperidinopropyl)carbamoyl-2-piperidone-5-carboxylates and analogs as elc antagonists)
179480-91-2 CAPLUS
5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-[[[3-[4-(4-etchyphonyl]-4-bunyl-1-piperidinyl)propyl)amino|carbonyl|-4-methyl-6-(4-nitrophenyl)-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:750506 CAPLUS
DOCUMENT NUMBER: 123:143638
ITILE: INVENTOR(S): 6luchowski, Charles Wetzel, Jo 123:143638 preparation of dihydropyridine derivatives as drugs Gluchowski, Charles: Wetzel, John M.: Chiu, George: Marzabadi, Mohammad R.: Wong, Wai C.: Nagerathnam,

Marzabadi, Mohammad K., Wong, wal C Dhanapalan Synaptic Pharmaceutical Corp., USA PCT Int. Appl., 760 pp. CODEN: PIXXID2 Patent English 2 PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

PAT					KIND DATE					APPL	ICAT	DATE							
	WO 9422829 WO 9422829				A2 19941013 A3 19950103					WO 1	994-	us38	52	19940405					
	W:															, GB,			
	RW:	AT,	BE.	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL	, UZ, , PT,			
AU	9464										MR, 994-					19940	405		
		360														19940 19960			
US	6211	198			B1		2001	0403		US 1	998-	9869	9			19980	615		
	6310	1076 11935			B1 A1		2001				2000- 2001-					20000 20011			
	6608	086			B2		2003	0819		,,e 1	003	4221	,			19930	405		
PRIORIT	API	LN.	INFO	.:							993-				λ	19930	910		
											1993- 1993-					19931 19931			
											994~					19940			
										US 1	1996- 1998 <i>-</i>	9869	9		A3	19960 19980	615		
										115 2	- ^ ^ ^	5889	79		רב	20000	เรกา		

MARPAT 123:143638

ANSWER 10 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

179480-95-6 CAPLUS
5-Pyrimidinecarboxylic acid, 1,2,3,4-tetrahydro-1-[[[3-[4-(4-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]amino]carbonyl]-4-methyl-6-(4-nitrophenyl)-2-oxo-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & & & \\ & \text{N} & & \text{(CH2)} \ 3-\text{NH}-\text{C}-\text{N} & \text{NH} \\ & & \text{O}_{2N} & & & \text{C}-\text{OHe} \\ \end{array}$$

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of 1-(4-arylpiperidinopropyl)carbamoyl-2-piperidone-5carboxylates and analogs as alc antagonists)
166809-56-9 CAPLUS

1000U9-36-9 CAPLUS 1-Piperidinepropanamine, 4-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN

AB Dihydropyridine derivs. [I: R1 - linear or branched alkyl, alkoxyalkyl, aralkyl: R2, R4 - H, linear or branched alkyl: R3 - H, linear or branched alkyl: R3 - H, linear or branched alkyl: alkoxyalkyl, acyl: R5, R6 - H, OH, C1 Br, F, NO2 CF3, cyano, NHZ, etc.: R7, R8 - H, cyano, CF3, CH, alkoxy, etc.: Y - C1-5 alkylene, C4-9 alkylene interrupted by O, alkenylene, alkynylene, etc.: Z - O. NH; CH2], useful in treating benign prostatic hyperplasia, inhibition of cholesterol synthesis, and reduction in intraocular pressure, are prepared and formulated.

Amidarlon of exchange and carbon of the control of the carbon of the carbon

Synthesis, and reduction in intraodular pressure, are prepared and unlated.

Amidation of carboxylic acid II (preparation given) with 3-(4,4-diphenylpiperidino)propylamine in refluxing CH2Cl2 gave 58.84 title compound (i)-III, which showed Ki of 1.9 nmol/kg in reducing urethral pressure in vivo in dogs.

166807-19-87 166807-35-89 166807-43-89
166807-19-29 166808-17-99 166808-19-19
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassificed); FRES (Preparation); USES (Uses)

[preparation of dihydropyridine derivs. as drugs)
166807-19-8 CAPLUS
3,5-8-yridinadicarboxamide, 2-ethyl-1,4-dihydro-N3-[3-[4-(4-methoxyphenyl)-4-henyl-1-piperidinyl]propyl]-6-methyl-4-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

• HCl

166807-35-8 CAPLUS
3,5-Pyridinedicarboxamide, 1,4-dihydro-N-[3-[4-(4-methoxyphenyl)-4-phenyl-piperidinyl]propyl]-2,6-dimethyl-4-(4-nitrophenyl)-, monohydrochloride
(9CI) (CA INDEX NAME)

166807-43-8 CAPLUS
3,5-Pyridinedicarboxamide, 2,6-diethyl-1,4-dihydro-N-[3-[4-(4-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-N'-methyl-4-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) (4-methoxyphenyl)-4-phenyl-1-piperidinyl]propyl]-6-methyl-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

166809-56-99
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dichydropyridine decive. as drugs)
166809-56-9 CAPIUS
1-Piperidinepropanamine, 4-(4-methoxyphenyl)-4-phenyl- (9CI) (CA INDEX NAME)

ANSWER 11 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

166807-47-2 CAPLUS
3,5-Pyridinedicarboxamide, N,2,6-triethyl-1,4-dihydro-N'-{3-{4-{4-methoxyphenyl}-4-phenyl-1-piperidinyl]propyl]-4-{4-nitrophenyl}- (9CI) (CA INDEX NAME)

166808-17-9 CAPLUS
3,5-Pyridinedicarboxamide, 2-[(2-azidoethoxy)methyl]-1,4-dihydro-N3-[3-[4-(4-methoxy)phenyl)-4-phenyl-1-piperidinyl]propyl]-6-methyl-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

166808-19-1 CAPLUS 3,5-Pyridinedicarboxamide, 2-[(2-aminoethoxy)methyl]-1,4-dihydro-N3-[3-[4-

L4 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:33860 CAPLUS
DOCUMENT NUMBER: 116:33860
TITLE: The metabolic fate of the antiparkinsonian drug budipine in rats
AUTHOR(S): Caputo, O.; Grosa, G.; Ceruti, M.; Rocco, F.; Biglino, G.

Caputo, O.; Gross, G.; Ceruti, M.; Rocco, F.; Biglino, G.
CORPORATE SOURCE: Ist. Chim. Farm. Appl., Univ. Torino, Turin, I-10125, Italy
SOURCE: European Journal of Drug Metabolism and Pharmacokinetics (1991), 16(2), 113-18
CODEN: EUROPD2; ISSN: 0398-7639
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The metabolic fate of the antiparkinsonian drug budipine was studied in rats after oral administration. The presence of an aromatic hydroxylation product, metabolite MI, and its O-sulfate conjugate was confirmed. Three new minor metabolites, budipine N-oxide, metabolite MI N-oxide, and a secondary metabolite decided from MI via hydroxylation of a Me of the tert-Bu group, were identified in urine. The presence of a metabolite, MI-glucuronic acid conjugate, was also established using different enzymic treatments of urine.

1 13936-43-1
RL: BPR (Biological process); RSU (Biological)

138306-43-1
RL: BPR (Biological process): BSU (Biological study, unclassified): BIOL (Biological study): PROC (Process) (pharmacokinetics of, as budipine metabolite)
138306-43-1 CAFLUS
1-Piperidineethanol, 4-(4-hydroxyphenyl)-β,β-dimethyl-4-phenyl-(9CI) (CA INDEX NAME)